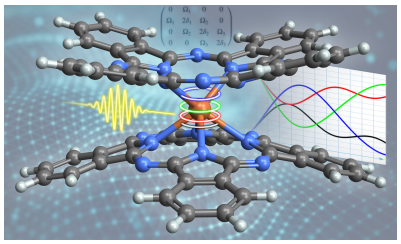
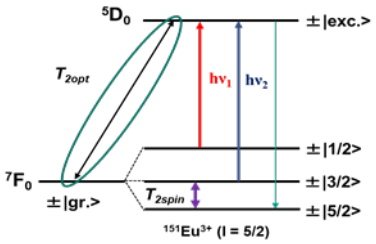
Open PhD position

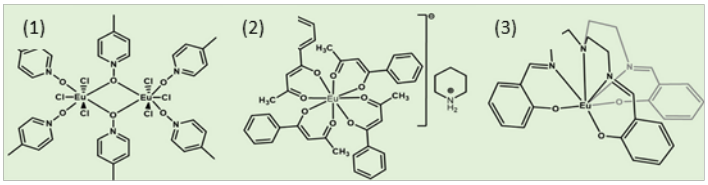
Title: Quantum State Engineering of Lanthanide Complexes for Optimally Controlled Quantum Information Processing



Nature **2012**, *488*, 357–360
Science **2014**, *344*, 1135-1138
Phys. Rev. Lett. **2017**,*119(18):* 187702
Nat. Commun. **2021**, *12*, 4443

Λ-systems for QIP





(2) Nature **2022,** *603, 241.*
(1) Nature Comms **2021,** *12*, 2152. *(3) J Phys Chem C* **2023,** *127*, 10670.

Type: Theory & programming

Short description: This project forms part of a collaboration with experimental chemists and physicists in Karlsruhe (KIT), with the aim of realizing quantum machine learning (QML) applications using Lanthanide complexes. Specifically, we focus on the theoretical modelling of higher-dimensional qu*d*its that arise from the nuclear spins (and the associated hyperfine interaction) of rare-earth atoms embedded in these molecules, which are read out electrically and/or optically. In the context of optimal Quantum Information Processing (QIP), the precise knowledge of the microscopic origin of the hyperfine interaction may open the way for the control and manipulation of the Hilbert-space topology of the quantum states. It can be performed by using physical means (e.g. applying a DC electric field or nuclear spin-photon interfaces) or chemical means (e.g. deformations of the ligands or substitution of a given lanthanide isotope by another one). This first line of research that we call **state engineering** requires the use of sophisticated methods of atomic/nuclear physics and quantum chemistry (e.g. Ligand-Field DFT). Moreover, individual hyperfine states can be addressed and manipulated using microwave electric pulses. The latter can be shaped using optimal control techniques for quantum optimization and will enable faster, more noise-robust or low-consumption logical gates. We call this second part of the project: **microwave pulse engineering**. The two parts are complementary.

The aim of this PhD work is to develop models using quantum chemical methods to tackle the state engineering part of the project. The microwave pulse engineering part will be developed in parallel by another PhD student.

Hosting institutions: KIT https://www.kit.edu/ and University of Strasbourg, Institute of Physics and Chemistry of Materials of Strasbourg (IPCMS) https://www.ipcms.fr/en/home/. This project is funded by the KIT. The duration is 4 years

Supervisors and email address: Prof. Paul-Antoine Hervieux, hervieux@unistra.fr and Prof. Mario Ruben, mario.ruben@kit.edu

Group websites: https://www.rubengroup.de/home.html &
https://www.ipcms.fr/en/equipe/theoretical-quantum-dynamics-of-nano-objects-dyno/

Eligibility requirements: We are looking for a highly motivated candidate with a master degree in quantum chemistry or theoretical physics. A strong background in quantum mechanics and computer simulations is required. Experience in molecular physics would be strongly appreciated. The candidate will have to collaborate cross-border and in a multidisciplinary context with partners working in quantum chemistry, materials chemistry and applied mathematics. Proficiency in English is also required. Good knowledge of Python and/or Mathematica and/or Matlab.

How to apply: Applicants should send a detailed CV (with references, i.e., names and email addresses of undergraduate and master internship supervisors), Master's report cards (M1 and M2 grades for applicants studying in French universities), and a letter of motivation to P. -A. Hervieux (hervieux@unistra.fr) and M. Ruben (mario.ruben@kit.edu).